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A PARAMETRIC STUDY OF THE RELEASE OF CO₂ IN SPACE

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1. INTRODUCTION

To conduct a meaningful experimental investigation in space, an understanding of the local environment prior to the experiment is required. There have been a number of attempts to describe the complex mixtures of gas at high altitudes and its effect on space shuttle sensors. Most of these earlier attempts have concentrated on the exhaust products of thruster motors and their collision with the atmosphere. Many of these investigations are described in a paper by Elgin, et.al., [1990]. The present work is based on simulations of a new comprehensive three-dimensional Monte Carlo code, SOCRATES (Spacecraft/Orbiter Contamination Representation Accounting for Transiently Emitted Species), which has been developed to account for contamination on spacecraft [Elgin and Sundberg, 1988]. In this investigation, the SOCRATES contamination-interaction code has been used to predict the reactions of CO₂ with atomic oxygen and hydrogen for altitudes of 500 to 800 km. This parametric study was undertaken to guide a future experiment for releasing CO₂ through a nozzle with a small diameter in the 500 to 800 km range altitudes. The atmospheric composition used in these calculations was taken from MSIS-86 [Hedin, 1987].

2. DESCRIPTION OF SOCRATES AND MSIS-86

The SOCRATES and MSIS-86 Models have been used for this investigation. The SOCRATES code is a comprehensive three-dimensional code and is based on the direct simulation Monte Carlo method [Elgin et al., 1990]. The principles and calculation techniques of direct simulation Monte Carlo method are extensively described by its originator [Bird, 1976]. It will briefly be described here. The solution region, a physical space, is a network of cells of different sizes. Initially, a discrete number of molecules are stored in the computer. These molecules are stored based on their velocity components, position coordinates, and other necessary information. The molecular motion and intermolecular collisions in the simulated region advance, and are modified with time, in a two stage process. In the first stage, the molecules advance along their trajectories according to their velocity components and the time increment. In this stage, some of the molecules may leave the solution domain and some will be introduced to the problem at hand according to the boundary conditions of the problem. In the second stage, a typical set of collisions will be simulated among the molecules in each cell with the appropriate time increment. The repetition of these two stages over the small time interval will uncouple the molecular motion and intermolecular collisions. The composition of the atmosphere was taken from the MSIS-86 Thermospheric Model [Hedin, 1987], which simulates the atmospheric environment at different altitudes.

2.1 THE SOCRATES CODE

In the SOCRATES code, the direct simulation Monte Carlo technique has been revised and extended significantly to account for the energy dependent collision cross sections [Bird, 1981] and a statistical collision model for internal energy effects [Borgnakke and Larsen, 1975] which have been described by Elgin and Sundberg [1988] and Elgin et al [1990]. In the code, the collision cross section is defined by the variable hard sphere model (VHS) which is a function of the relative velocity between two molecules. The collision cross section can be stated as

$$\sigma = \sigma_{\text{ref}} \left(\frac{v_r}{v_{\text{ref}}} \right)^{-2\omega} \quad (1)$$

where σ_{ref} and v_{ref} are the reference collision cross section and velocity, respectively [Elgin, et.al., 1990]. ω is a constant parameter which has a value of 0.25 for this investigation.

2.1.1 Reactive Collisions

Reactive collisions between molecules and/or atoms (which is relevant to the present work) can be simulated directly by SOCRATES. The reaction cross section is a function of the relative collision energy as defined by Equation (1). The Monte Carlo program, in the event of collision, simulates the reaction with a probability which is related to the ratio of the reactive to collision cross section at the relative velocity for the collision [Elgin and Sundberg, 1988].

The present work employs the option of using the Arrhenius rate constant in the code to calculate the reactive collision cross section. The rate constant has the form of

$$k_r = A T^n e^{-\frac{E_a}{R_0 T}} \quad (2)$$

where A and n are constant parameters, R_0 and T are gas constant and temperature, respectively, and E_a is the activation energy. In the case of the collision between two reactants, the reaction cross section is calculated, and the reaction is counted with a weighting factor W_r . The weighting factor is given by

$$W_r = W_c \frac{v_r \sigma^*}{v_r \sigma} \quad (3)$$

where σ^* , σ , and W_c are the previous collision cross section, collision cross section, and collision weighting factor, respectively. Further discussion of the reactive collisions can be found in the report by Elgin and Sundberg [1988].

2.2 THE MSIS-86 MODEL

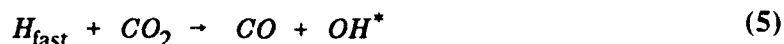
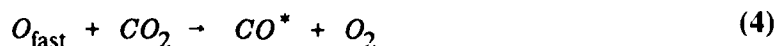
MSIS-86 is an empirical model for calculating the temperature, density, and composition of the atmospheric environment at altitudes of 85 to 1000 kilometers. The model is based on the data from several satellites, numerous rocket probes, and ground based incoherent scatter stations [Hedin, 1987]. At a given altitude, geomagnetic condition and solar condition, data such as atmospheric density, composition, and atmospheric temperature, are obtained from the model.

3. DESCRIPTION OF THE CONFIGURATION MODEL

A nozzle with a small diameter is assumed to be the source of CO_2 gas released into space from a space platform. The diameter of the nozzle and mass flow rate of the CO_2 remain constant. It is assumed that the gas release will last approximately 10 seconds. The angle of attack refers to the angle between the velocity vector and the centerline of the gas plume, and is exactly 180° since the gas plume is assumed to be released directly into RAM. The temperature of the CO_2 gas at the time of release is assumed to be about 50°C . The solution region for an unsteady case (only reaction 4 is considered) is taken to be a cubic space 15.6 km^3 in volume ($2.5 \times 2.5 \times 2.5 \text{ km}^3$) consisting of 6480 unevenly spaced cells, with 8 molecules in each cell. The solution domain in a steady state case (for both reactions) is taken to be a cubic space 29.25 km^3 in volume ($3.25 \times 3.0 \times 3.0 \text{ km}^3$) consisting of 8400 unevenly spaced cells. In each cell there are 6 molecules for each species.

4. DISCUSSION OF RESULTS

The reactions of CO₂ with atomic oxygen and hydrogen are:



The asterisk denotes vibrational excitation.

The reaction of CO₂ with atomic oxygen is endothermic by 0.33 electron volts and at orbital velocity, at 180° collision angle, it has excess energy of 4 electron volts. The simulation for the reaction CO₂ and O for the altitudes of 500 to 800 km are presented in two cases of unsteady and steady state conditions. However, for the reaction CO₂ and H, only the steady state condition has been considered. Tables 1-4 represent the parameters used for the simulation. Figures 1-3 and 6 show plots of total intensity and molecular flux as a function of time and altitude after release. Figures 4, 5, and 7 show a panel of gray scale plots for the radiation intensity of CO and OH vibrational excitation in steady state condition for different altitudes.

Table 1 shows the reference collision cross-section, reference relative collision velocity, and number of internal degrees of freedom for the species. Table 2 shows the values used in Arrhenius Rate Coefficients for the different reactions.

TABLE 1. Molecular Parameters Used in the Calculations

Species	σ_{ref} cm ⁻²	V_{ref} cm/s	v_i
O	1.75×10^{-15}	2.49×10^5	0.00
CO	3.46×10^{-15}	2.09×10^5	2.00
O ₂	3.17×10^{-15}	1.98×10^5	3.60
CO ₂	4.33×10^{-15}	1.71×10^5	3.58
H	1.03×10^{-15}	1.09×10^6	0.00
OH	1.77×10^{-15}	8.00×10^5	2.00

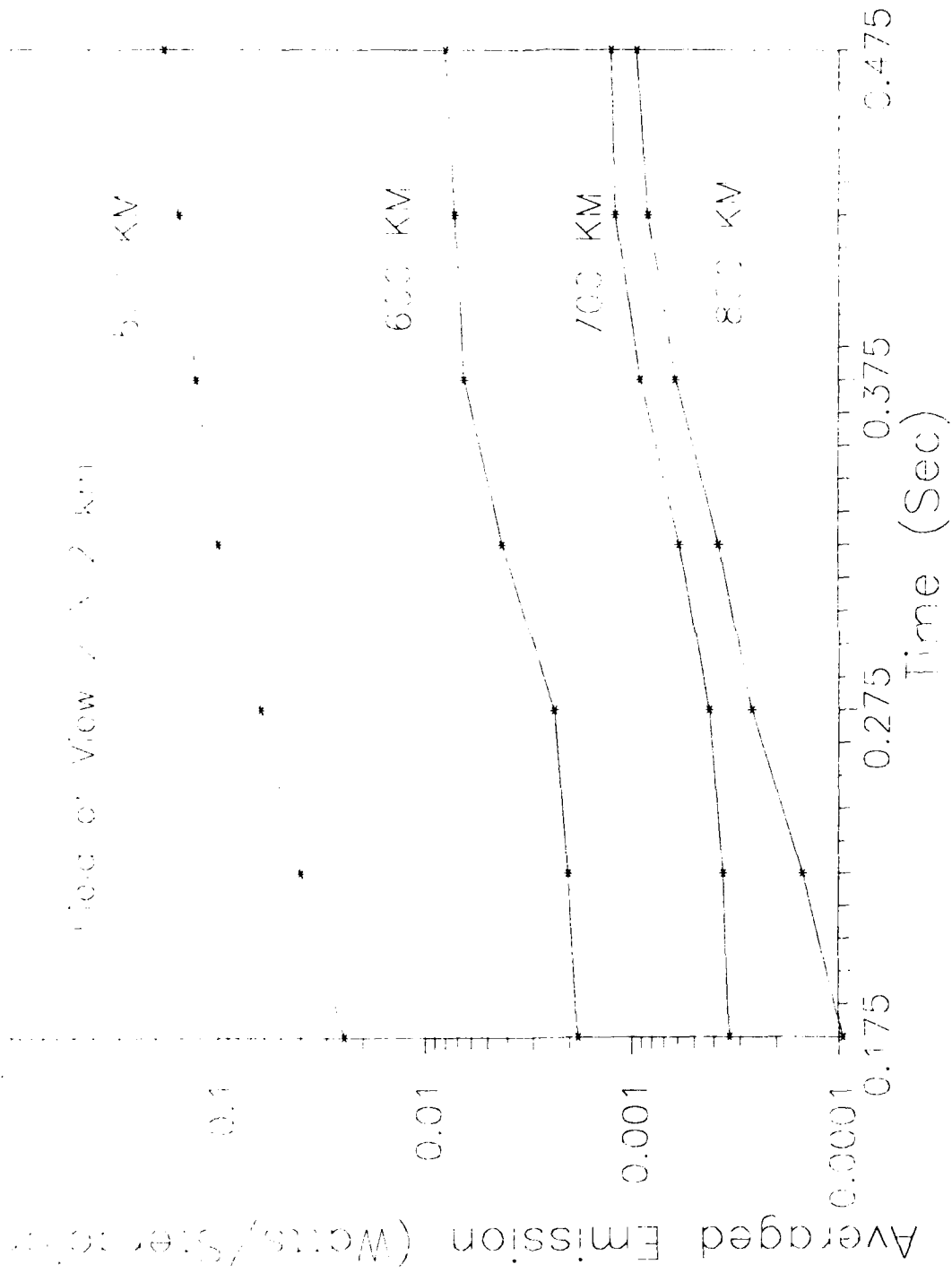


Figure 1. Total Solution Region Averaged Values For CO^* Vibrational Excitation in Unsteady State Condition

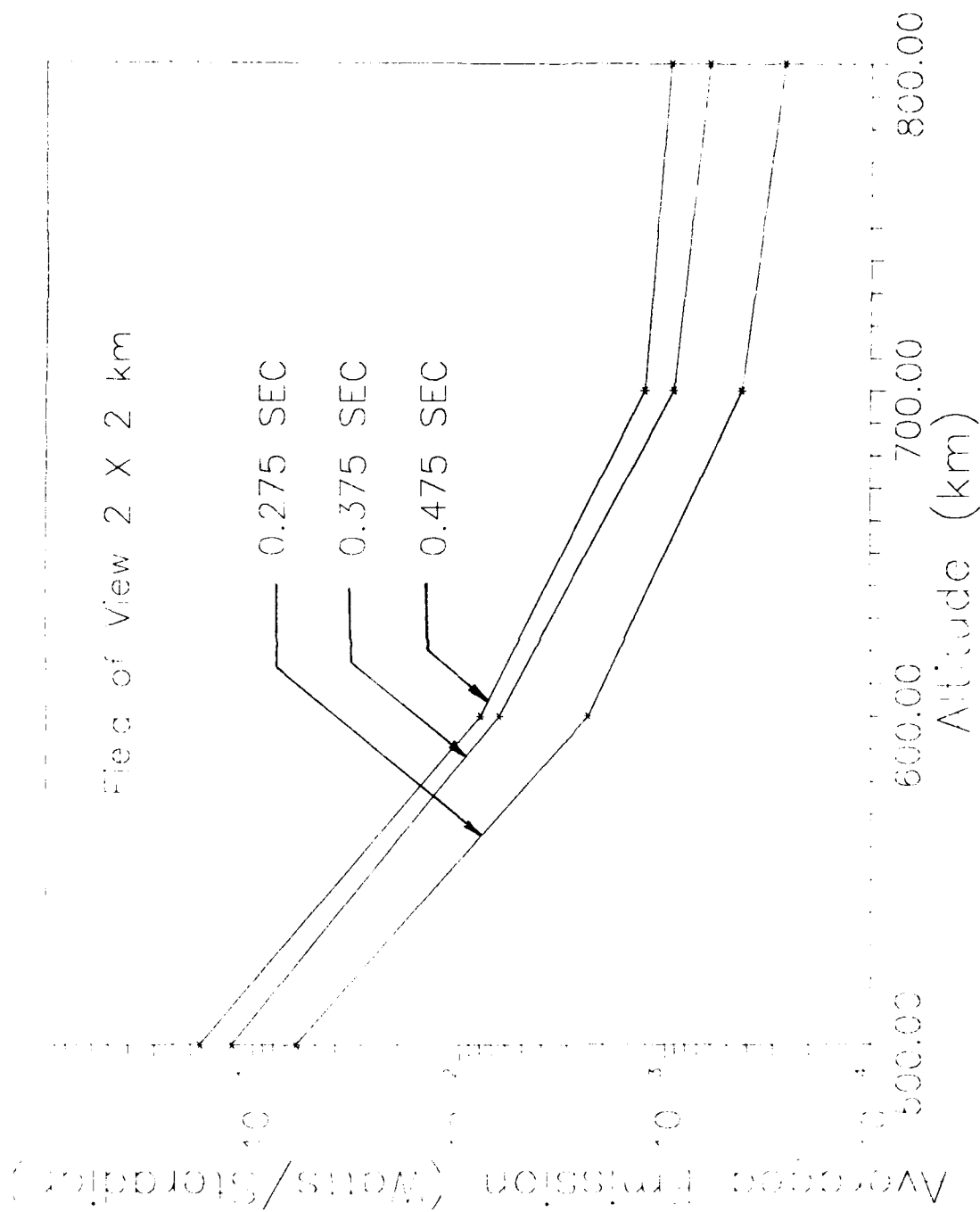


Figure 2. Total Solution Region Averaged Values Versus Altitude For CO₂ Radiation Solution

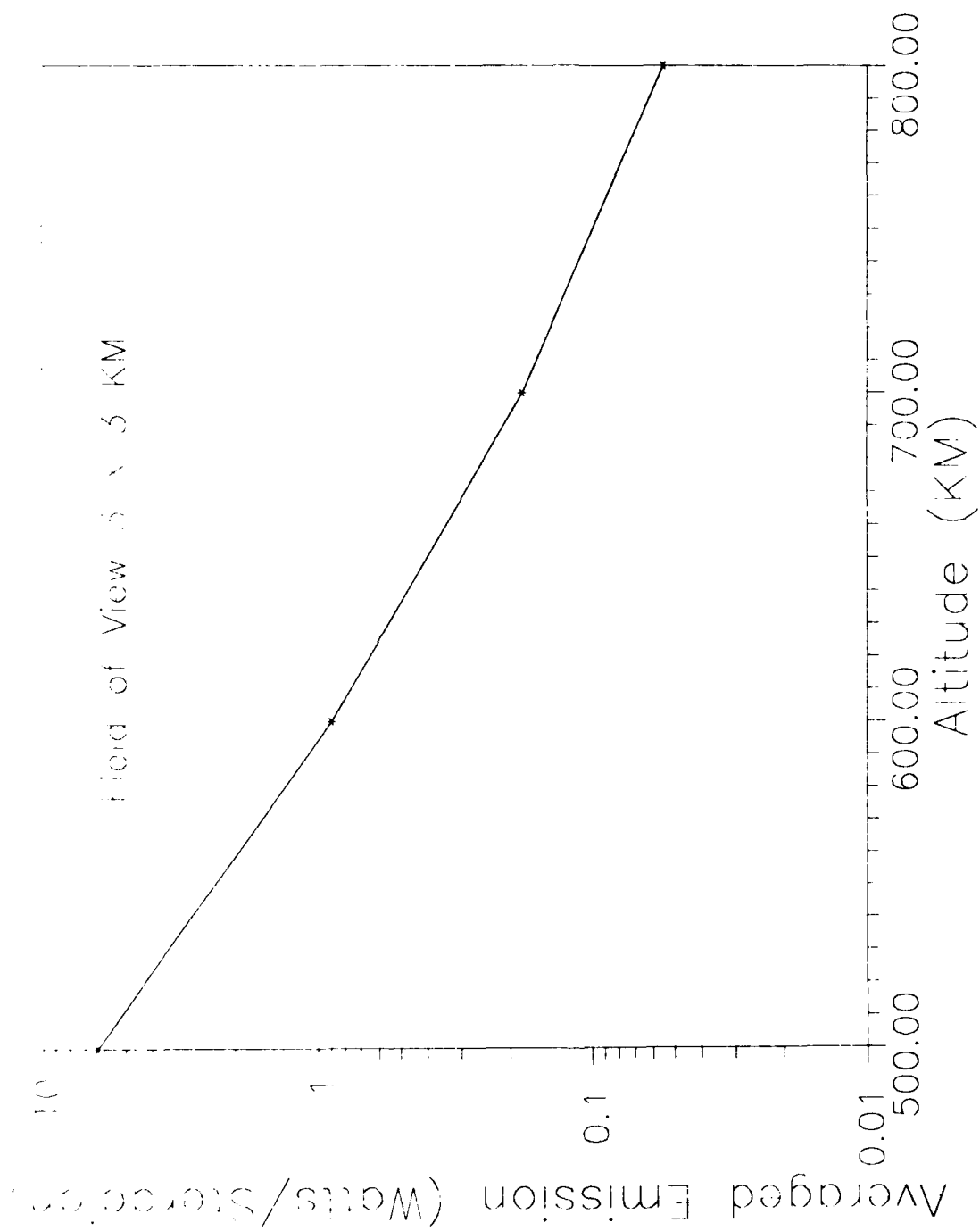


Figure 3. Total Soution Region Averaged Values For CO⁺ Vibrational Excitation

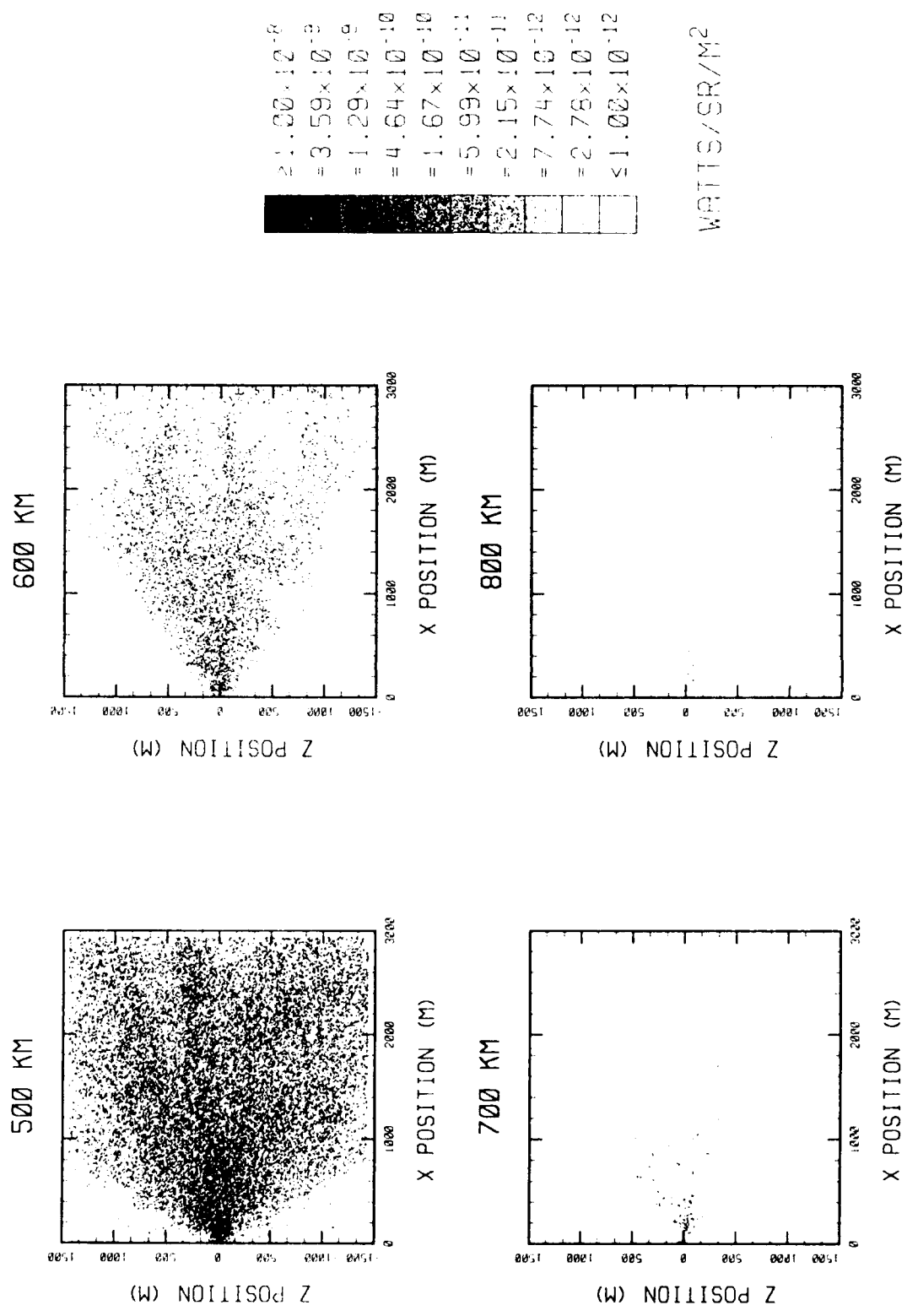


Figure 4. Gray Scale plots showing the CO Vibration-rotation emission at 4.6 μm from the Voyager 1 mission at 500, 600, 700, and 800 km altitudes.

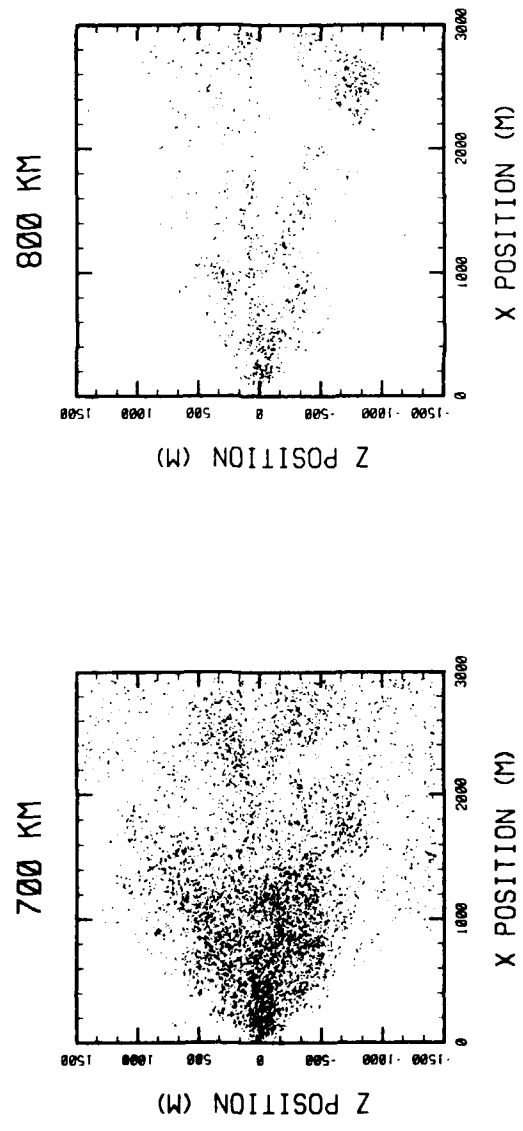
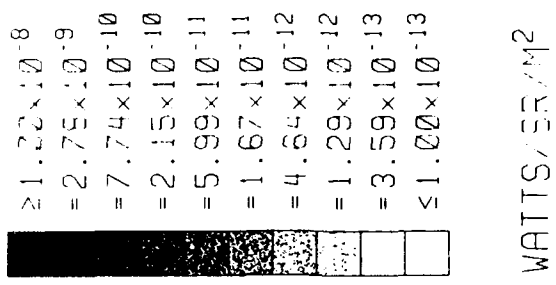
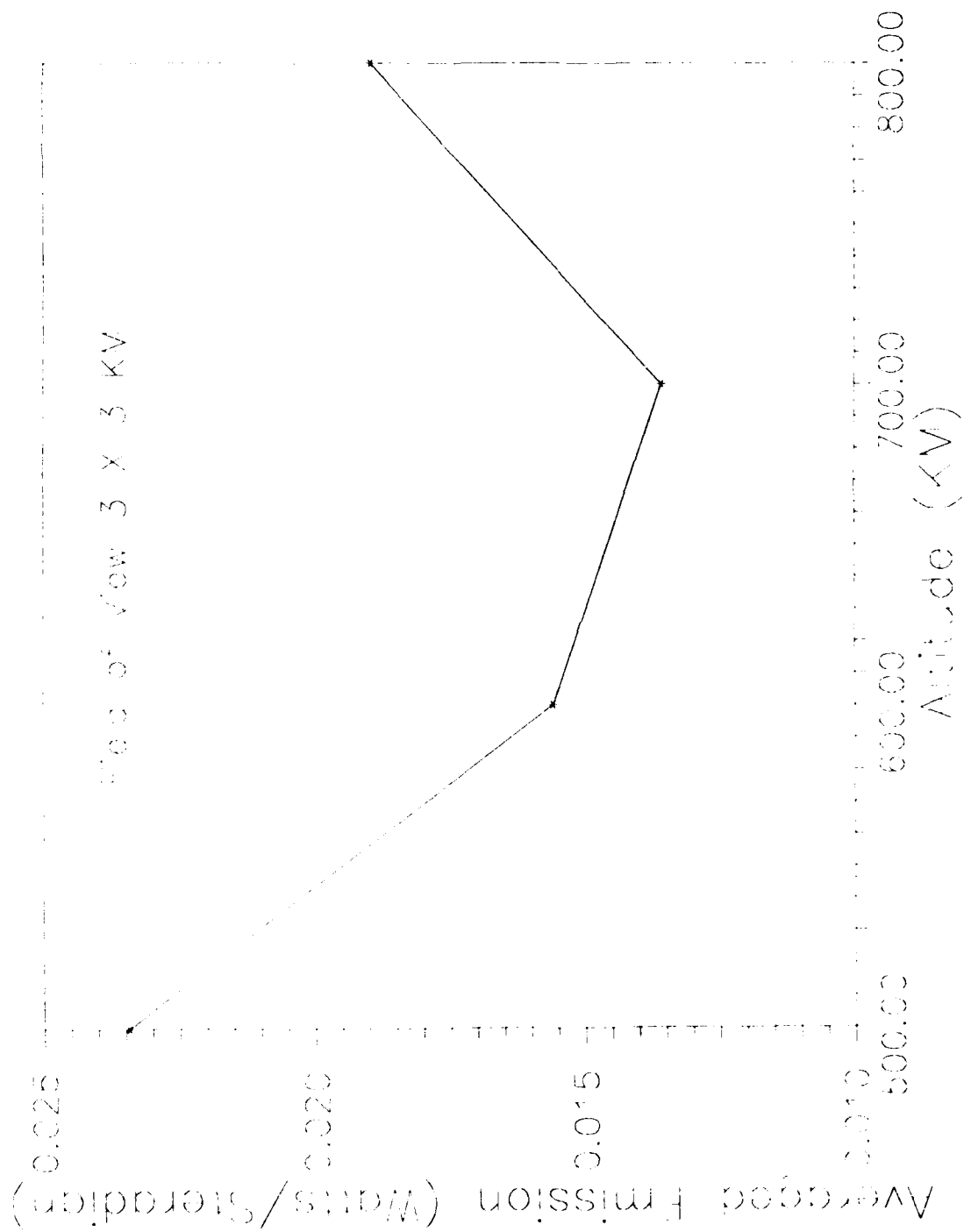


Figure 5. Gray Scale Plots Showing the CO Vibrational Emission at $4.6 \mu\text{m}$ from the Mechanism $\text{C} + \text{CO}_2 \rightarrow \text{CO} + \text{C}$



Altitude (KV) after Radio Averaged Values for 3 X 3 View of View 3 X 3 KV

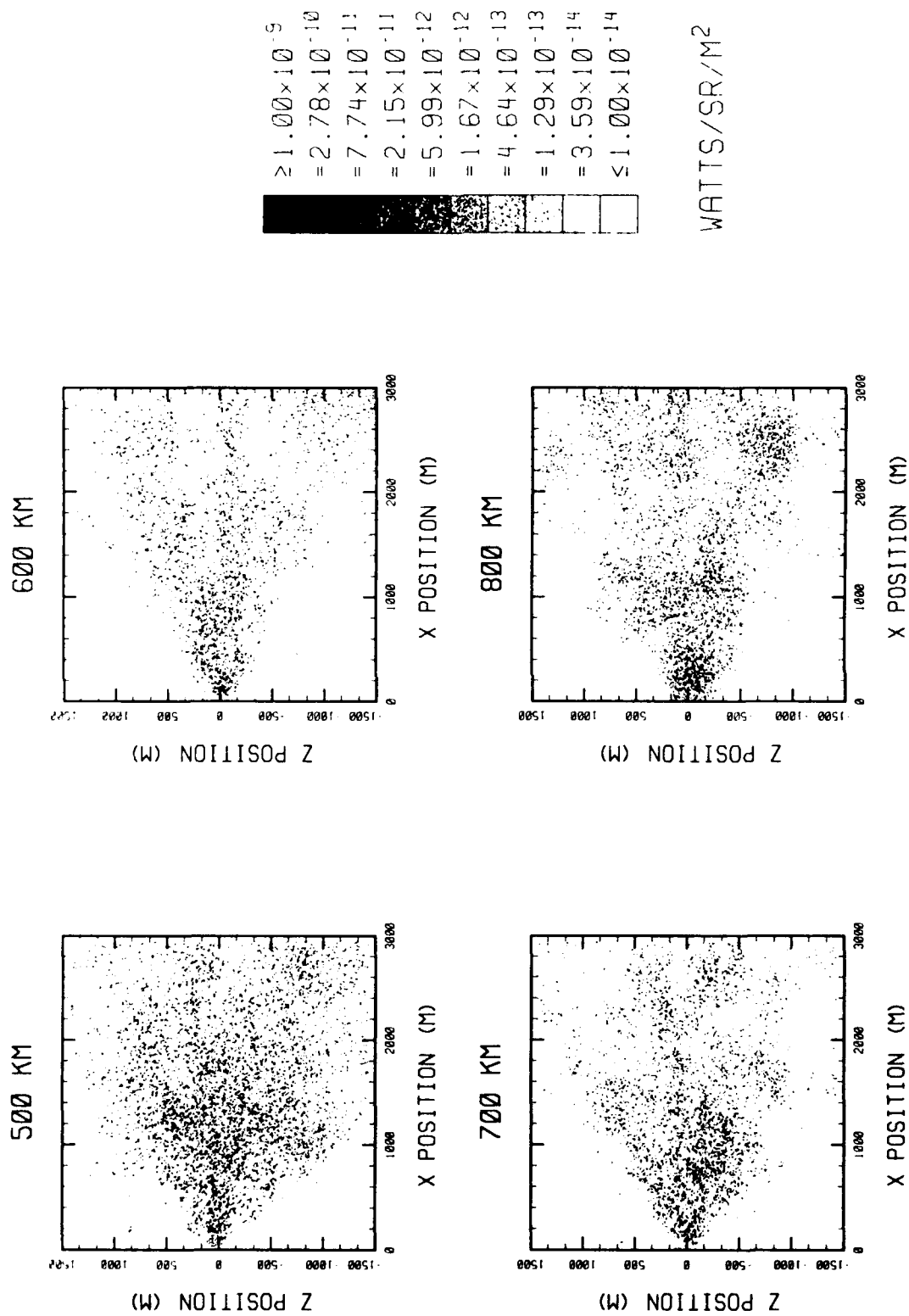


Figure 7. Gray Scale Plots Showing the OH Vibrational Emission at 2.7 μm from the Mechanism $\text{H} + \text{CO}_2 \rightarrow \text{OH}^* + \text{CO}$

TABLE 2. Rate Coefficient Used in SOCRATES, $k = AT^n \exp(-E_a/kT)$

Reaction	A	n	E_a (kcal/mole)	ΔH (kcal/mole)
$O_{fast} + CO_2 \rightarrow CO^* + O_2$	2.0(-11)	0.0	14.3	14.3
$H_{fast} + CO_2 \rightarrow CO + OH^*$	2.5(-10)	0.0	13.3	13.3

Table 3 shows the results of the MSIS-86 model simulation for atmospheric density and temperature for the altitudes of 500 to 800 km. The code was run for some typical condition in late 1993 (the proposed date for the experiment).

TABLE 3. Atmospheric Density and Temperature

Altitude (km)	Number density (cm^{-3})	Temperature ($^{\circ}K$)
500	2.735×10^7	1002.2
600	8.437×10^6	1002.3
700	3.652×10^6	1002.3
800	2.080×10^6	1002.3

It should be mentioned here that the unsteady simulation for CO_2 with O is considered to be up to 0.5 sec. However, it required 7.26 sec for both emissions from Reactions 4 and 5 to reach a steady state condition. The total averaged emission values for Figures 1, 2, and 3 are at the wavelength of $4.6 \mu m$ and are in terms of watts/steradian. The vibrational frequency of OH (Figure 6) is $2.7 \mu m$. The field of view for Figures 1 and 2 is about 2 by 2 km and for Figures 3 and 6 is 3 by 3 km.

Table 4 lists the other parameters that have been used in SOCRATES to simulate CO_2 released from a 5 mm diameter nozzle with a mass flow rate of 100 g/s. Figure 1 shows the total averaged emission from the mechanism of $O + CO_2 \rightarrow CO^* + O_2$ (Reaction 4) for an unsteady state condition in the time range of 0.175 to 0.475 sec. The amounts of emission at altitudes of 700 and 800 km are close to each other in Figure 1. However, at altitudes of 500 and 600 km, the emission is almost on an order of 100 and 10 higher, respectively, when compared to the reaction emission for the 700 or 800 km altitude. Figure 2 shows the total averaged emission as a function of altitude and, as expected, there is a sharp drop in the emission from 500 to 700 km altitude. However, there is no

significant change from the 700 to 800 km altitude. Figure 3 shows the total averaged emission for the steady state condition as a function of altitude. As it can be seen from the figure, there is a significant increase in the amount of radiation in steady state conditions compared to the unsteady state case (Figure 2). Figure 4 shows a panel of gray scale plots for the radiation intensity of Reaction 4 at different altitudes, from 10^{-8} to 10^{-12} watts/m²/sr. The figure shows that there is a sharp decrease in CO⁺ radiation when going from 500 km to 800 km altitude. Figure 5 shows a similar situation for CO radiation, but only for 700 and 800 km altitudes at a range of 10^{-8} to 10^{-13} watts/m²/sr. Figure 6 shows the total averaged emission from the mechanism of $H + CO_2 \rightarrow OH + CO$ (Reaction 5) for steady state conditions. As can be seen from the figure, the amount of reaction emission for 800 km is much more intense than the reaction emission for the 600 and 700 km altitudes. This is due to the increased H atoms density at 800 km, compared with that at 600 or 700 km. This is shown in Figure 7, where the radiation at 2.7 μ m (OH fundamental wavelength) is plotted for altitudes 500 to 800 km.

TABLE 4. Parameters Used in the Simulations for a 5 mm nozzle diameter

Parameter	Value
Mass Flow	100.0 g/s
Exit Plane Area	2.0×10^{-1} cm ²
Ratio of Specific Heat	1.30
Exit Mach Number	3.53
Exit Nozzle Half Angle	8.00 degrees
Exit Plane Density	0.005092 g/cm ³
Exit Plane Number Density	6.969×10^{19} molecules/cm ³
Exit Plane Velocity	1.0 km/s
Exit Plane Speed of Sound	2.833×10^4 cm/s
Exit Plane Temperature	326.7° K
Exit Plane Pressure	3.143×10^6 dynes/cm ²
Stagnation Temperature	937.3° K
Stagnation Pressure	3.027×10^8 dynes/cm ²
Thrust	23.86 lb
Velocity of Spacecraft	7.4 km/s

5. SUMMARY AND CONCLUSIONS

A bundle of CO_2 gas was assumed to be released from a nozzle with a small diameter at high altitude. The diameter of nozzle and mass flow rate are assumed to be 5 mm and 100 g/s, respectively, in this parametric investigation. The reactions $\text{O} + \text{CO}_2 \rightarrow \text{CO}^* + \text{O}_2$ and $\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}^*$ were simulated for the above cases from altitudes of 500 to 800 km, using the contamination-interaction code SOCRATES, and the MSIS-86 Thermospheric model. The results were presented in forms of graphs and gray scale plots for these simulations. The total averaged emission for the reaction of CO_2 and O for a field of view of approximately 2 by 2 km in an unsteady condition was calculated as a function of time and altitude. In the steady state condition, both reactions were considered. They are represented by the total averaged emissions versus altitude and intensity of radiation in gray scale plots. These simulations show that the radiation from these reactions can be measurable for the parameters which have been used in these calculations.

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